

Table 26.1. List of published structures for supplementary exercises organized by complexity

N	Chemical Formula	Space Group	V, Å ³	N _{atm} ¹	N _{dis} ²	N _H ³	Comments
<i>Simple</i>							
1	VO(CH ₃ COO) ₂	Cmc2 ₁	670	6			
2	WO ₂ (O ₂)(OH ₂)	P2 ₁ /n	335	6			
3	ε-VOPO ₄	P2 ₁ /n	328	7			
4	Al ₂ (OH) ₃ VO ₄	C2/m	547	8			
5	MnV ₂ O ₅	Pnma	394	8			
6	NaB(C ₂ O ₄) ₂	Cmcm	657	8			
<i>Medium</i>							
7	WO ₂ (O ₂)(OH ₂)·1.66H ₂ O	C2/m	431	6			Partial occupation of water
8	VO(OCH ₂ CH ₂ O)	C2/c	860	10		4	Positioning of H atoms
9	Au _{0.75} Ni _{0.25} OSn ₄	Ccca	473	3	1		Mixed site occupation
10	K _{0.27} MnO ₂ ·0.54H ₂ O	R-3m	151	4	1		Mixed site occupation

¹ Total number of atoms in the asymmetric unit cell. ² Number of disordered sites. ³ Number of located H atoms.

Table 26.1. List of published structures for supplementary exercises organized by complexity (*continue*)

N	Chemical Formula	Space Group	V, Å ³	N _{atm} ¹	N _{dis} ²	N _H ³	Comments
11	LiB(C ₂ O ₄) ₂	Pnma	637	11			Pseudo-hexagonal cell ^a
12	Zn ₃ (OH) ₂ (V ₂ O ₇)·2H ₂ O	P-3m1	228	7		1	Locating of H atom
13	HIO ₃	P2 ₁ 2 ₁ 2 ₁	264	5		1	Charge flipping solution
<i>Complex</i>							
14	Li _{2x} V _{1-x} O _{2-x} ·0.5H ₂ O, x=1/6	I4/mmm	217	5	3		Heavy atom method
15	[N(CH ₃) ₄]Mo ₄ O ₁₂	C2/m	1435	13			Complex structure and PO ^b
16	(CH ₃ NH ₃) _{0.75} V ₄ O ₁₀ ·0.67H ₂ O	C2/m	468	10	3		Significant disorder
17	[V _{7,2} O ₈ (OH) ₈](Cl) _{0.77} (H ₃ O) _{2.3}	I4/m	329	7	4	1	Significant disorder
18	[N(CH ₃) ₄]V ₈ O ₂₀	C2/m	523	11			Disordered intercalated ion
19	Mo _{5.25} O _{17.25} ·(H ₂ O) _{1.4}	P6 ₃ /m	358	5	3		Pseudo-cubic cell ^a
20	(NH ₄) _{0.94} Mo _{5.29} O _{17.29}	P6 ₃ /m	362	6	4		Significant disorder

¹ Total number of atoms in the asymmetric unit cell. ² Number of disordered sites. ³ Number of located H atoms.
^a Cell parameters ratio suggests higher symmetry than the actual symmetry of the structure. ^b Preferred orientation.